

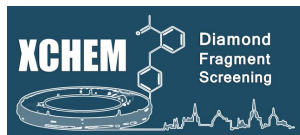
Diamond Light Source

ORN's first external Virtual Environment

Tim Dudgeon (IM)

on behalf of

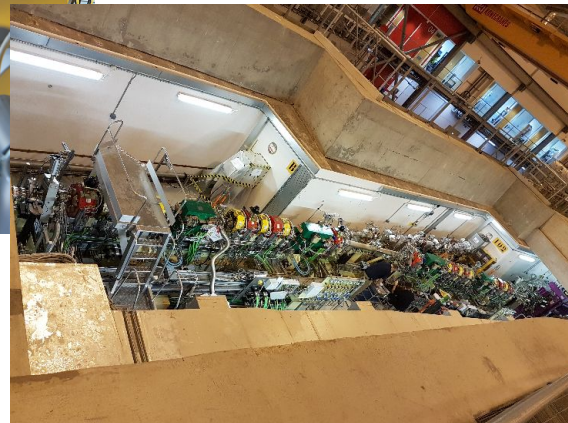
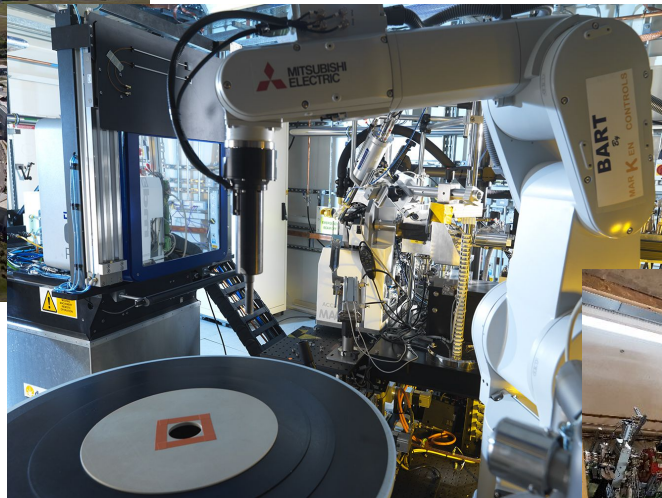
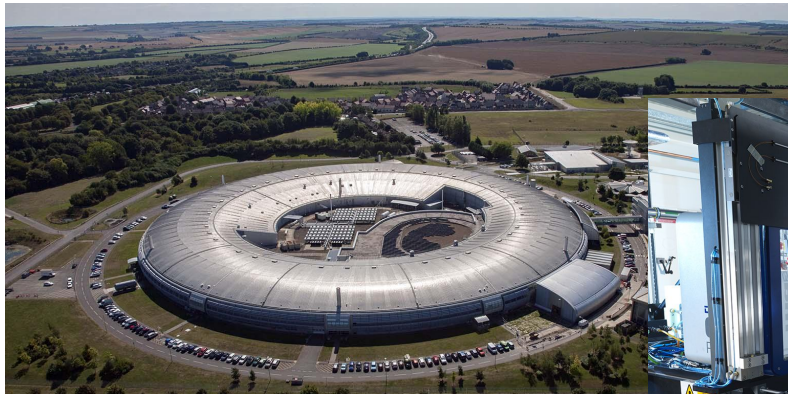
Frank von Delft, Rachael Skyner



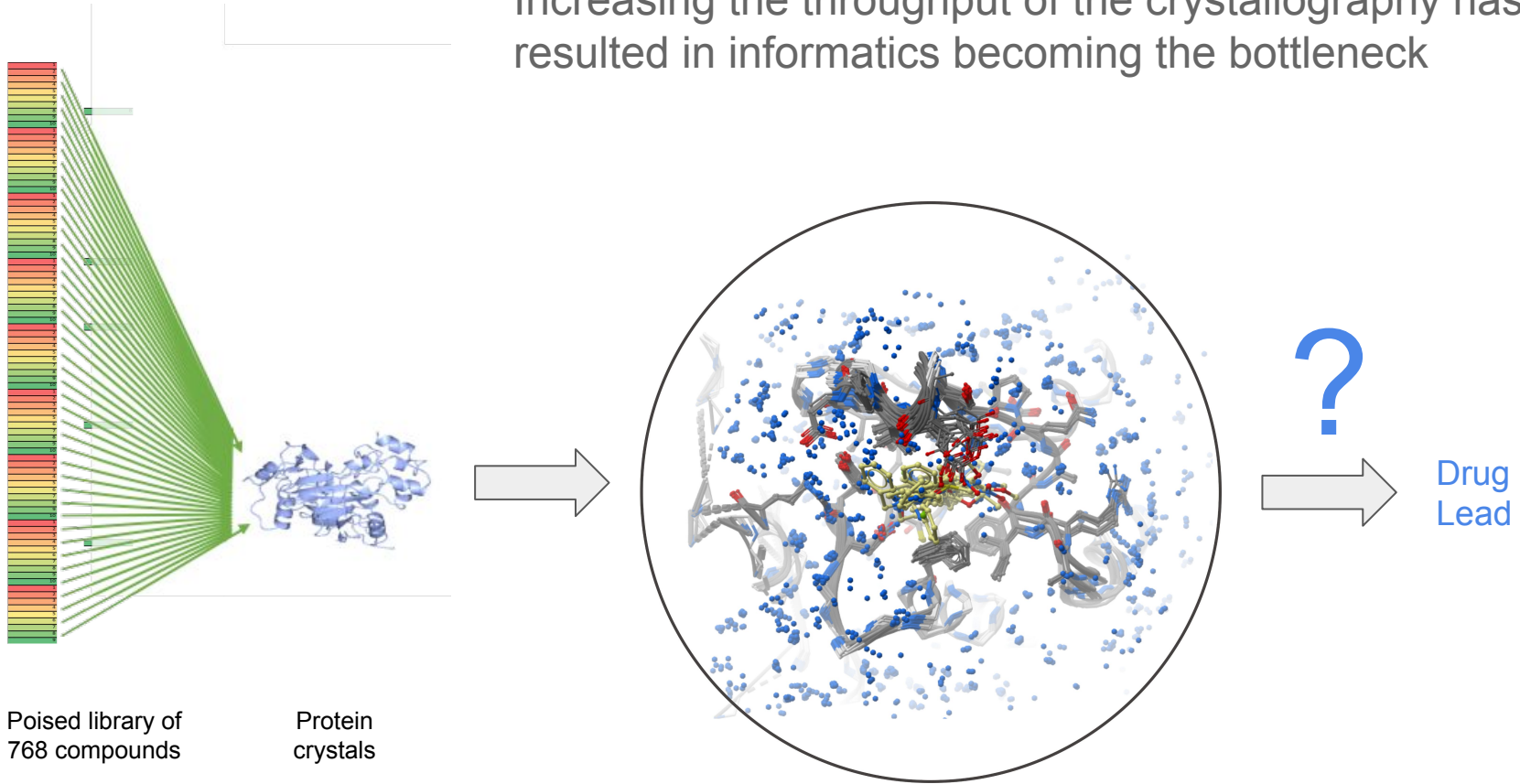
diamond



Fragment screening at Diamond

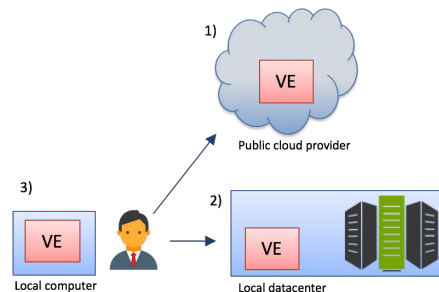
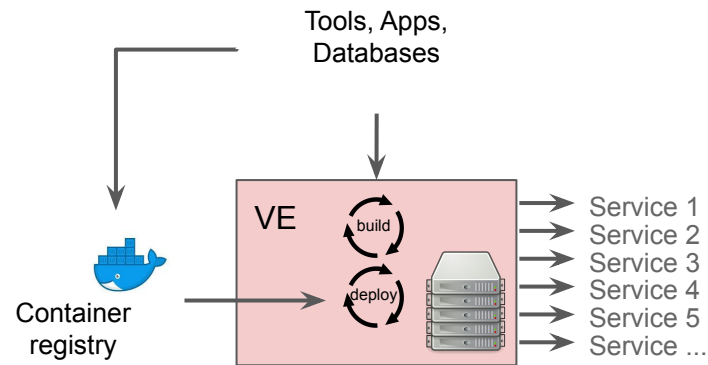


Increasing the throughput of the crystallography has resulted in informatics becoming the bottleneck



Why an OpenRiskNet Virtual Environment?

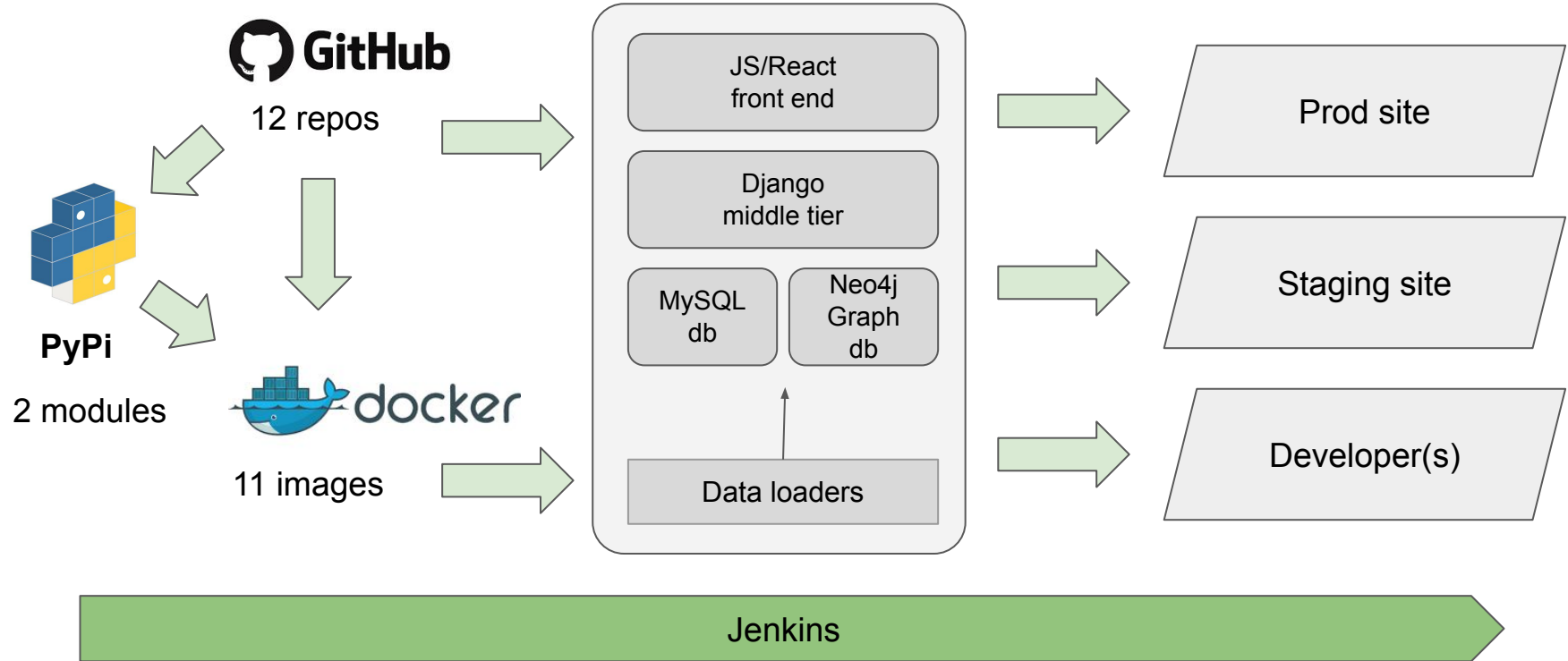
- Existing solution - no need to develop
- Built on robust platform (OpenShift/Kubernetes)
- Support/expertise available locally (IM)
- Availability of ORN applications (Squonk, ADMET predictions)
- Allows to deploy Diamond specific apps
- CI/CD process

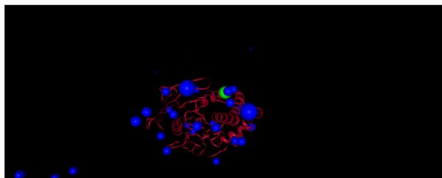


The Diamond VE

- Running on 'bare metal' OpenStack cluster (*IroniC*) on Verne Global cloud in Iceland
 - 1 Bastion
 - 1 Master node - 4 cores, 32GB RAM
 - 1 Infra node - 20 cores, 128GB RAM
 - 1 Worker node- 20 cores, 128GB RAM
 - 1 HiMem node - 20 cores, 512GB RAM (for Neo4j graph database)
 - 1 GPU node (little used so far)
- OpenShift cluster deployed using the standard ORN deployment tools
 - Including some of the ORN applications
- This cluster interacts with computing facilities and data at Diamond and STFC (both on Harwell Campus)

Core app stack - Fragalysis: <https://fragalysis.diamond.ac.uk>



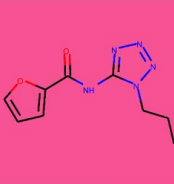



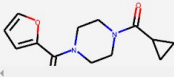
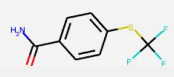
Molecule Cluster Selector

On 13 of a total of 52

Previous

Next

	
PTP1B-g0193	PTP1B-g0766
Undefined	Undefined
Ligand	Ligand
Complex	Complex
Vectors	Vectors

	
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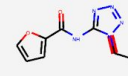
Viewer controls

Change background colour

Number picked: 0
Number vectors explored: 0
Number series explored: 0
Estimated cost: £0

Download CSV (Chrome)

Download Yank/Duck

Selected Interaction: **Not selected**

Compounds to pick. Mol total: 68

Select All

Clear Selection

Blue Red Green Purple Apricot



Ongoing work

- Integration with HPC (docking, MD techniques)
 - Workflow tool integration (Squonk, Galaxy)
 - PySquonk
- Application enhancements
- Improve deployment (for Pharma)
 - Simplify and streamline
 - Better customisation
- Work being planned to at least end 2020

PySquonk

- Python modules that:
 - Allow access computational services from Squonk
 - Docking
 - Property prediction/filtering
 - Other cheminformatics and comp chem tools
 - In future ADMET tools and predictions
 - Will be integrated into Fragalysis
 - Exemplified using Jupyter notebooks
- Work being done as part of the ORN implementation challenge
 - Expected to be complete by end November

Summary

- The ORN VE was a natural choice for Diamond
- OpenShift/Kubernetes provides a powerful and flexible platform for deploying scientific applications
- CI/CD processes have been critical
- Establishes a route for uptake of ORN VE by pharma
- Work continues!